



**U.S. Department of Energy  
Energy Efficiency and  
Renewable Energy**

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## INDUSTRIAL TECHNOLOGIES PROGRAM

# Advances in Process Intensification through Multifunctional Reactor Engineering

## Novel Reactor Concept Promises Increased Efficiency

Process intensification is a key strategy that the chemical industry is adopting for increasing energy efficiency and profitability. Multifunctional reactors (i.e., chemical reactors that integrate other functions such as separations) form the cornerstone of process intensification. Catalytic distillation is the classic example of multifunctional reaction engineering. However, no multiphase catalytic reactors currently operate in the novel mode that is the subject of this project, and no three-phase (vapor/liquid/liquid) commercial reactors exist for this mode. Existing systems are oversized and operate at less than optimal efficiency.

The novel multiphase catalytic reactor designs that result from this project will offer the chemical industry significant improvement in energy efficiency and process performance through enhanced mass and heat transfer. The technology will allow for optimization of existing trickle-bed reactors, such as refinery hydrotreaters. Other processes that could benefit include those that utilize liquid catalysts such as phosphoric acid, nitric acid, or ionic liquids. Applications that could benefit include 1) higher capacity vapor/liquid catalytic downflow reactors with fixed-bed catalyst systems, 2) vapor/liquid/liquid reactors in which the catalyst is one

of the liquid phases or is contained in one of the liquid phases, and 3) vapor/liquid upflow reactors utilizing a homogeneous catalyst slurry.

### Multifunctional Reactor



*Over the last decade, Sandia's Slurry Bubble-Column Reactor (SBCR) testbed has been successfully used to support indirect liquefaction studies.*

**Sandia's Slurry Bubble-Column Reactor (SBCR) testbed**



### Benefits for Our Industry and Our Nation

- Potential energy savings of 83 trillion Btu per year by 2020
- Fuel and electricity savings of at least 50%
- Improved reactor performance through more efficient mass and heat transfer
- Significantly reduced solid wastes through reduction in acid used for alkylation

### Applications in Our Nation's Industry

The process is being developed specifically for acid catalyzed C4 paraffin/olefin alkylation. However, these novel multiphase catalytic reactors could be used in other processes across the chemical industry. In particular, processes that use liquid catalysts such as phosphoric acid, nitric acid, or ionic liquids will enjoy significant improvements in performance and efficiency.

### Project Partners

Chemical Research and Licensing Company  
Pasadena, TX

ABB Lummus  
Houston, TX

Sandia National Laboratories  
Albuquerque, NM

## Project Description

**Goal:** The overall objective of the project is to develop the knowledge and tools required to develop and scale a novel multiphase, catalytic reactor for acid catalyzed C4 paraffin/olefin alkylation to industrial dimensions.

The focus of the project will be on the sulfuric-acid-catalyzed C4 paraffin/olefin alkylation reaction, which is a key process area in which to obtain energy savings via efficient mixing of fluids. An efficient system would obtain high mass transfer between the process liquids by utilizing a novel flow regime as opposed to impeller mixing devices.

Experiments have demonstrated that the proposed mode of operation in vessels containing structured packing material can enhance inter-phase mass transfer. Important physical phenomena occurring in this environment include evaporation, condensation, mass transfer between the phases, chemical reactions, heat release and transfer, and three-phase flow through a structured material. Normally in this process, the interaction between the hydrocarbon liquid and the acid phase limits reaction rate, while the absence of effective fluid/fluid contact leads to the formation of undesired heavier molecular weight. The novel mode of operation overcomes these negative effects with less energy expenditure than the traditional approach of using high-shear mixers.

### Activities:

This project will consist of interrelated experimentation (bench-scale and pilot-scale) and modeling tasks. The bench-scale experiments will focus on materials characterization, process chemistry, and structure-scale hydrodynamics. The pilot-scale experiments will focus on vessel-scale hydrodynamics. Project partners will also investigate the transition between trickle-flow and other modes and the characteristics of the changes. They will develop detailed models of structure-scale processes, which they will incorporate into a vessel-scale hydrodynamics model.

### Milestones

#### Year 1:

- 1) Simulant system for pilot-scale experiment
- 2) Bench-scale hydrodynamics experiment
- 3) Pilot-scale pulse-flow hydrodynamics experiment

#### Year 2:

- 1) Validated model of bench-scale hydrodynamics
- 2) Initial data sets from pilot-scale experiments

#### Year 3:

- 1) Model of pilot-scale hydrodynamics
- 2) Comprehensive pilot-scale data set showing benefits
- 3) Validation of scaling approach
- 4) Final report documenting validated scale-up approach
- 5) Transition to commercial-scale design

## For additional information, please contact:

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## A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

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